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 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  MAY 01  New CAS web site launched
 NEWS  3  MAY 08  CA/CAplus Indian patent publication number format defined
 NEWS  4  MAY 14  RDISCLOSURE on STN Easy enhanced with new search and display
                  fields
 NEWS  5  MAY 21  BIOSIS reloaded and enhanced with archival data
 NEWS  6  MAY 21  TOXCENTER enhanced with BIOSIS reload
 NEWS  7  MAY 21  CA/CAplus enhanced with additional kind codes for German
                  patents
 NEWS  8  MAY 22  CA/CAplus enhanced with IPC reclassification in Japanese
                  patents
 NEWS  9  JUN 27  CA/CAplus enhanced with pre-1967 CAS Registry Numbers
 NEWS 10  JUN 29  STN Viewer now available
 NEWS 11  JUN 29  STN Express, Version 8.2, now available
 NEWS 12  JUL 02  LEMBASE coverage updated
 NEWS 13  JUL 02  LMEDLINE coverage updated
 NEWS 14  JUL 02  SCISEARCH enhanced with complete author names
 NEWS 15  JUL 02  CHEMCATS accession numbers revised
 NEWS 16  JUL 02  CA/CAplus enhanced with utility model patents from China
 NEWS 17  JUL 16  CAplus enhanced with French and German abstracts
 NEWS 18  JUL 18  CA/CAplus patent coverage enhanced
 NEWS 19  JUL 26  USPATFULL/USPAT2 enhanced with IPC reclassification
 NEWS 20  JUL 30  USGENE now available on STN
 NEWS 21  AUG 06  CAS REGISTRY enhanced with new experimental property tags
 NEWS 22  AUG 06  BEILSTEIN updated with new compounds
 NEWS 23  AUG 06  FSTA enhanced with new thesaurus edition
 NEWS 24  AUG 13  CA/CAplus enhanced with additional kind codes for granted
                  patents
 NEWS 25  AUG 20  CA/CAplus enhanced with CAS indexing in pre-1907 records
 NEWS 26  AUG 27  Full-text patent databases enhanced with predefined
                  patent family display formats from INPADOCDB
 NEWS 27  AUG 27  USPATOLD now available on STN
 NEWS 28  AUG 28  CAS REGISTRY enhanced with additional experimental
                  spectral property data

 NEWS EXPRESS  29 JUNE 2007:  CURRENT WINDOWS VERSION IS V8.2,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

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FILE 'HOME' ENTERED AT 11:47:08 ON 30 AUG 2007

=> FIL HCAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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FILE COVERS 1907 - 30 Aug 2007 VOL 147 ISS 10
FILE LAST UPDATED: 29 Aug 2007 (20070829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s isoflavone
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          5686 ISOFLAVONES
L1        8261 ISOFLAVONE
               (ISOFLAVONE OR ISOFLAVONES)

=> s l1 and process
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       1687760 PROCESSES
       3698879 PROCESS
                (PROCESS OR PROCESSES)
L2         545 L1 AND PROCESS

=> s l2 and 2-hydroxydeoxybenzoin
       9272756 2
            57 HYDROXYDEOXYBENZOIN
            26 HYDROXYDEOXYBENZOINS
            67 HYDROXYDEOXYBENZOIN
                (HYDROXYDEOXYBENZOIN OR HYDROXYDEOXYBENZOINS)
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             21 2-HYDROXYDEOXYBENZOIN
                (2(W)HYDROXYDEOXYBENZOIN)
L3            1 L2 AND 2-HYDROXYDEOXYBENZOIN

=> s l1 and 2-hydroxydeoxybenzoin
        9272756 2
             57 HYDROXYDEOXYBENZOIN
             26 HYDROXYDEOXYBENZOINS
             67 HYDROXYDEOXYBENZOIN
                (HYDROXYDEOXYBENZOIN OR HYDROXYDEOXYBENZOINS)
             21 2-HYDROXYDEOXYBENZOIN
                (2(W)HYDROXYDEOXYBENZOIN)
L4           13 L1 AND 2-HYDROXYDEOXYBENZOIN

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        4428017 ACID
        1589146 ACIDS
        4930039 ACID
                (ACID OR ACIDS)
            101 ANYDRIDE
              9 ANYDRIDES
            108 ANYDRIDE
                (ANYDRIDE OR ANYDRIDES)
              0 FORMIC ACID ANYDRIDE
                (FORMIC(W)ACID(W)ANYDRIDE)
L5            0 L4 AND FORMIC ACID ANYDRIDE

=> s l4 and process
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        1687760 PROCESSES
        3698879 PROCESS
                (PROCESS OR PROCESSES)
L6            1 L4 AND PROCESS

=> s l4 base
MISSING OPERATOR L4 BASE
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s l4 and base
         721462 BASE
         160847 BASES
         818445 BASE
                (BASE OR BASES)
L7           3 L4 AND BASE

=> d his

     (FILE 'HOME' ENTERED AT 11:47:08 ON 30 AUG 2007)

     FILE 'HCAPLUS' ENTERED AT 11:47:33 ON 30 AUG 2007
L1         8261 S ISOFLAVONE
L2          545 S L1 AND PROCESS
L3            1 S L2 AND 2-HYDROXYDEOXYBENZOIN
L4           13 S L1 AND 2-HYDROXYDEOXYBENZOIN
L5            0 S L4 AND FORMIC ACID ANYDRIDE
L6            1 S L4 AND PROCESS
L7            3 S L4 AND BASE
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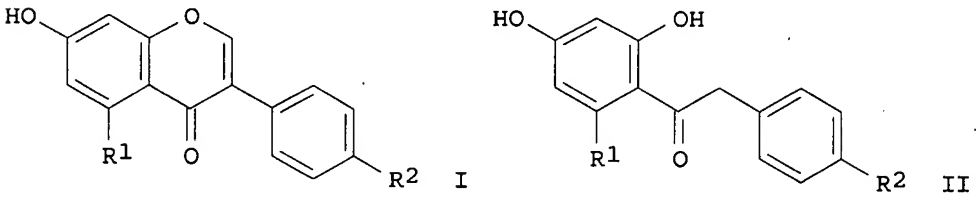
=> d l3 ibib abs hitstr tot

L3 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:80674 HCAPLUS
DOCUMENT NUMBER: 140:128190
TITLE: Process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivatives
INVENTOR(S): Burdet, Bruno; Ruettimann, August
PATENT ASSIGNEE(S): Roche Vitamins Ag, Switz.; DSM IP Assets B.V.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009576	A2	20040129	WO 2003-EP7575	20030714
WO 2004009576	A3	20040513		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2492201	A1	20040129	CA 2003-2492201	20030714
AU 2003254341	A1	20040209	AU 2003-254341	20030714
EP 1523478	A2	20050420	EP 2003-764976	20030714
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003012840	A	20050426	BR 2003-12840	20030714
CN 1684950	A	20051019	CN 2003-817676	20030714
JP 2005534682	T	20051117	JP 2004-522445	20030714
MX 2005PA00795	A	20050419	MX 2005-PA795	20050119
US 2005256321	A1	20051117	US 2005-521972	20050121

PRIORITY APPLN. INFO.: EP 2002-16494 A 20020723
WO 2003-EP7575 W 20030714

OTHER SOURCE(S): CASREACT 140:128190; MARPAT 140:128190
GI



AB The present invention discloses a process for manufacturing hydroxylated isoflavone derivs., such as I [R1 = H, OH; R2 = OH,

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=> s l1 sss full
FULL SEARCH INITIATED 12:18:09 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     92168 TO ITERATE

100.0% PROCESSED     92168 ITERATIONS                                 1 ANSWERS
SEARCH TIME: 00.00.01

L3             1 SEA SSS FUL L1

=> FIL HCAPLUS
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     172.10     172.31

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FILE COVERS 1907 - 30 Aug 2007  VOL 147 ISS 10
FILE LAST UPDATED: 29 Aug 2007  (20070829/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> s l3
L4             9 L3

=> FIL REGISTRY
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       7.80     180.11

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DICTIONARY FILE UPDATES:  29 AUG 2007  HIGHEST RN 945828-45-5

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alkoxy] by reacting an appropriately substituted 2-hydroxydeoxybenzoin derivs. II with formic acid anhydride, HCOOCOR3 [R3 = alkyl, haloalkyl, alkoxymethyl, carboxyalkyl, arylalkyl, cycloalkyl, aryl, heteroaryl, aminoalkyl, alkoxy, aryloxy], in the presence of a base or in a solvent which acts as a base, and if necessary promoting the ensuing hydrolysis of the so-produced acylated form of I by acidification. Of particular interest as products of this process are the 5,7-dihydroxyisoflavones, e.g. genistein I [R1, R2 = OH (III)]. Thus, propionyl formic anhydride, formed by the reaction of sodium formate and propionyl chloride, was reacted with II [R1, R2 = OH], and the product was hydrolyzed to afford III of 98.9% purity. Isoflavones display many useful biochem. effects.

=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:674200 HCAPLUS
DOCUMENT NUMBER: 145:505229
TITLE: A convenient method of isoflavone synthesis
AUTHOR(S): Aitmambetov, A.; Tlegenov, R. T.; Tokhtybaeva, A. M.
CORPORATE SOURCE: Complex Institute of Natural Sciences, Karakalpak Division, Academy of Sciences of Uzbekistan, Nukus, 742000, Uzbekistan
SOURCE: Russian Journal of Bioorganic Chemistry (2006), 32(4), 400-401
CODEN: RJBCET; ISSN: 1068-1620
PUBLISHER: Pleiades Publishing, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:505229
AB Reaction of 2-hydroxydeoxybenzoins with bis(dimethylamino)methane in ethanol results in isoflavonones.
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:80674 HCAPLUS
DOCUMENT NUMBER: 140:128190
TITLE: Process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivatives
INVENTOR(S): Burdet, Bruno; Ruettimann, August
PATENT ASSIGNEE(S): Roche Vitamins Ag, Switz.; DSM IP Assets B.V.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009576	A2	20040129	WO 2003-EP7575	20030714
WO 2004009576	A3	20040513		

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PL, PT, RO, RU, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ,
UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
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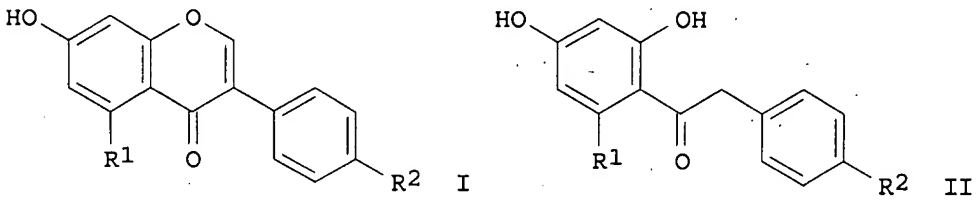
CA 2492201	A1	20040129	CA 2003-2492201		20030714
AU 2003254341	A1	20040209	AU 2003-254341		20030714
EP 1523478	A2	20050420	EP 2003-764976		20030714
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
BR 2003012840	A	20050426	BR 2003-12840		20030714
CN 1684950	A	20051019	CN 2003-817676		20030714
JP 2005534682	T	20051117	JP 2004-522445		20030714
MX 2005PA00795	A	20050419	MX 2005-PA795		20050119
US 2005256321	A1	20051117	US 2005-521972		20050121
PRIORITY APPLN. INFO.:			EP 2002-16494	A	20020723
			WO 2003-EP7575	W	20030714

OTHER SOURCE(S): CASREACT 140:128190; MARPAT 140:128190
GI



AB The present invention discloses a process for manufacturing hydroxylated isoflavone derivs., such as I [R1 = H, OH; R2 = OH, alkoxy] by reacting an appropriately substituted 2-hydroxydeoxybenzoin derivs. II with formic acid anhydride, HCOOCOR3 [R3 = alkyl, haloalkyl, alkoxymethyl, carboxyalkyl, arylalkyl, cycloalkyl, aryl, heteroaryl, aminoalkyl, alkoxy, aryloxy], in the presence of a base or in a solvent which acts as a base, and if necessary promoting the ensuing hydrolysis of the so-produced acylated form of I by acidification. Of particular interest as products of this process are the 5,7-dihydroxyisoflavones, e.g. genistein I [R1, R2 = OH (III)]. Thus, propionyl formic anhydride, formed by the reaction of sodium formate and propionyl chloride, was reacted with II [R1, R2 = OH], and the product was hydrolyzed to afford III of 98.9% purity. Isoflavones display many useful biochem. effects.

L4 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:81319 HCAPLUS
DOCUMENT NUMBER: 114:81319
TITLE: Synthesis and anabolic action of modified isoflavones
AUTHOR(S): Vasil'ev, S. A.; Golubushina, G. M.; Kabachnyi, V. I.; Lukyanchikov, M. S.; Molchanov, G. I.; Sokolovskaya, T. I.; Khilya, V. P.
CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1990), 24(9), 38-41
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal

LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 114:81319
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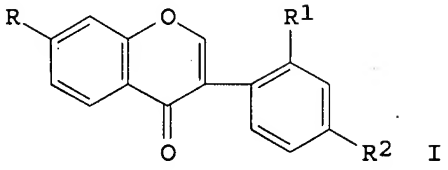

I

AB Isoflavones I (R = R2 = H, R1 = H, F; R = R1 = H, R2 = F) (II) were prepared in 95-98% yields by treating the corresponding 2-hydroxydeoxybenzoins with POCl3-DMF catalyzed by BF3.Et2O. Treating II with Me2CHI gave 92-96% I (R = Me2CH); treating II with PhCH:CHCOCl gave 79% I (R = PhCH:CHCO). Addnl. obtained was 95% I (R = CHMeCO2Me, R1 = F, R2 = H; R1 = H, R2 = F). Anabolic activity of I in rats was studied.

L4 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:128778 HCAPLUS
DOCUMENT NUMBER: 92:128778
TITLE: Synthesis of insecticidal diphenylisoxazole derivatives
AUTHOR(S): Szabo, Vince; Nemeth, Laszlo; Borda, Jeno; Bokor, Gyorgy
CORPORATE SOURCE: Alkalmazott Kem. Tansz., Kossuth Lajos Tudomanyegy., Debrecen, Hung.
SOURCE: Magyar Kemiai Folyoirat (1979), 85(9), 385-7
CODEN: MGKFA3; ISSN: 0025-0155
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
OTHER SOURCE(S): CASREACT 92:128778
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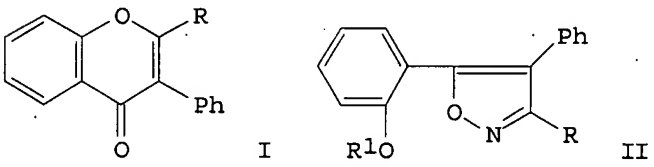

I II

AB Isoflavones I (R = H, Me, CF3), prepared from 2-hydroxydeoxybenzoin by Claisen condensation and Kostanecki-Robinson acylation, resp., were treated with NH2OH in aqueous EtOH at pH 8 to give 80-95% II (R1 = H), which were treated either with R2NCO (R2 = Me, Et, Bu) to give II (R1 = CONHR2), or with (EtO)2PSCl to give II [R1 = P(S)(OEt)2].

L4 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:441861 HCAPLUS
DOCUMENT NUMBER: 89:41861
TITLE: Base-catalyzed transformation of a β-dicarbonyl acetal, 1-(2-hydroxyphenyl)-2-phenyl-3,3-

dimethoxypropan-1-one into isoflavone and 2-hydroxydeoxybenzoin
AUTHOR(S): Zsuga, M.; Szabo, V.; Balogh, L.
CORPORATE SOURCE: Inst. Appl. Chem., Lajos Kossuth Univ., Debrecen, Hung.
SOURCE: Reaction Kinetics and Catalysis Letters (1978), 8(1), 1-6
CODEN: RKCLAU; ISSN: 0133-1736
DOCUMENT TYPE: Journal
LANGUAGE: English
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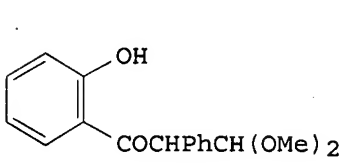

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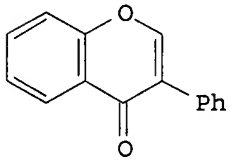

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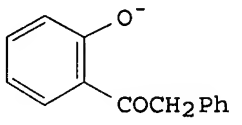

III

AB The decomposition of I depends on the OH- concentration At [OH-] ≤10-3M. I transforms into II, while at [OH-] = 10-2M, it decomps. to III via an enol-enolate equilibrium These unusual base-catalyzed transformations are explained by the high mobility of the α-proton of I, and by the stability of II towards nucleophilic reagents.

L4 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:479033 HCAPLUS
DOCUMENT NUMBER: 83:79033
TITLE: Synthesis of C-3-substituted chromones. I. New condensing agent for isoflavone synthesis by Claisen condensation
AUTHOR(S): Szabo, Vince; Borbely, Szabolcs; Farkas, Erzsebet; Tolnai, Sandor
CORPORATE SOURCE: Alkalmazott Kem. Tansz., Kossuth Lajos Tudomanyegyetem, Debrecen, Hung.
SOURCE: Magyar Kemiai Folyoirat (1975), 81(5), 220-4
CODEN: MGKFA3; ISSN: 0025-0155
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
OTHER SOURCE(S): CASREACT 83:79033
GI For diagram(s), see printed CA Issue.
AB Optimal parameters of the Claisen condensation, leading to isoflavone I (R = H, MeO; R1 = H, Me, MeO; R2 = H, OH, MeO; R3 = H, MeO) were determined The reaction is homolog-independent and differences exist only in the ease of product isolation. Me3CONa is more convenient and safer than Na as condensing agent and provides 5-40% higher yields.

L4 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:405631 HCAPLUS
DOCUMENT NUMBER: 75:5631
TITLE: Synthesis of C-2 substituted isoflavones

AUTHOR(S): Szabo, V.; Farkas, Mrs. E.; Levai, A.
CORPORATE SOURCE: Alk. Kem Tansz., Kossuth Lajos Tud. Egy., Debrecen, Hung.
SOURCE: Acta Physica et Chimica Debrecina (1970), 15/16, 191-9
CODEN: APDBAN; ISSN: 0567-7947
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Baker-Venkataraman transformation of 2-hydroxydeoxybenzoin acetates (I, R = Ac; R1 = OAc; R2 = H; R3 = H, OAc; R4 = H, NO2) and α-acetoxyhydroxystilbene acetates (II, R1 = OAc; R2 = H; R3 = H, OAc; R4 = H, NO2) by hot aqueous alc. NaOH, absolute alc. NaOEt at room temperature, and hot absolute NEt3, resp., into 2-methylisoflavones (III, R = Me; R1 = OH, OAc; R2 = H; R3 = H, OH, AcO; R4 = H, NO2) was investigated. A significant difference in the yields of III from I and II, resp., was found only if the reaction mixture contained H2O. Kostanecki-Robinson acylation of hydroxydeoxybenzoins (I, R = H; R1 = H, OH; R2 = H, Me; R3 = H, OH; R4 = H, OH, MeO, NO2) with (RCO)2O (R = Me, Et, iso-Pr, Ph) in the presence of NEt3 or N-ethylpiperidine was also useful for preparation of III.

L4 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1969:524127 HCAPLUS
DOCUMENT NUMBER: 71:124127
TITLE: Synthesis of some isoflavones
AUTHOR(S): Le-Van-Thoi; Nguyen-Van-Hoang
CORPORATE SOURCE: Lab. Org., Fac. Sci., Saigon, S. Vietnam
SOURCE: Vietnamica Chimica Acta (1966) 87-100
CODEN: VICABS; ISSN: 0372-5863
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB Deoxybenzoins I, where one of R, R1, R2 is OH, are treated with HCO2Et and Ac2O to give isoflavones II. Thus, a mixture of 10 g. PhCH2CO2Ph and 6.3 g. AlCl3 is heated 3 hrs. at 140° to give 60% 2-hydroxydeoxybenzoin (III), m. 55°, 2,4-dinitrophenylhydrazone m. 214-15°, and 10% 4-hydroxydeoxybenzoin. Similarly prepared are (m.p., % yield, and m.p. 2,4-dinitrophenylhydrazone given): I (R = OH, R2 = Me, R1 = H), 65°, 80, 218°; I (R = OH, R1 = Me, R2 = H) (b5 164°), -, 50, 235°. III (0.60 g.) in 30 ml. HCO2Et is added to powdered Na at -10°; the mixture is kept 20 hrs. at 0° and 40 hrs. at room temperature to give 0.30 g. isoflavone, m. 130°. Similarly prepared are the following II (R, R1, R2, and m.p. given): Me, H, H, 136°; H, H, Me, 169°; Me, H, Me, 90°; H, Me, H, 108°; Me, Me, H, 89°.

L4 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1958:113686 HCAPLUS
DOCUMENT NUMBER: 52:113686
ORIGINAL REFERENCE NO.: 52:20142f-i,20143a-c
TITLE: The synthesis of isoflavones
AUTHOR(S): Gowan, J. E.; Lynch, M. F.; O'Connor, N. S.; Philbin, E. M.; Wheeler, T. S.
CORPORATE SOURCE: Univ. Coll., Dublin, Ire.
SOURCE: Journal of the Chemical Society (1958) 2495-9
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 52:113686

AB Isoflavones have been obtained by the action of formanilide or formamide on benzyl o-hydroxyphenyl ketones (2-hydroxydeoxybenzoins). It was necessary to protect the OH group in the deoxybenzoins, except that in the 2-position. A mixture of 50 g. AlCl3, 24 g. p-dimethoxybenzene, 24 g. phenylacetyl chloride and 200 ml. Et2O was refluxed 8 hrs. and worked up to give 16 g. benzyl 2-hydroxy-5-methoxyphenyl ketone, m. 45° (ligroine, b. 40-60°). The following ketones (deoxybenzoins) were prepared by conventional methods, but other than those given for them in the literature: benzyl 2,4-diacetoxyphenyl, m. 135-6° (HOAc); benzyl 2,4-dibenzoyloxyphenyl, m. 110-12° (HOAc); 2-hydroxy-4-methoxyphenyl 4-nitrobenzyl, m. 134-6° (EtOH); 2-hydroxy-4,6-dimethoxyphenyl 4-nitrobenzyl, m. 150° (EtOH); benzyl 2-hydroxy-4,5-dimethoxyphenyl, m. 93° (EtOH). The following new ketones (deoxybenzoins) were prepared: 2-benzyloxyphenyl benzyl, m. 94° (EtOH); benzyl 2-cinnamoyloxyphenyl, m. 99° (EtOH); benzyl 2-hydroxy-4-p-nitrobenzoyloxyphenyl, m. 178-80° (EtOH); benzyl 2-hydroxy-4-p-toluenesulfonyloxyphenyl, m. 117° (EtOH); 4-benzoyloxy-2-hydroxyphenyl 4-methoxybenzyl, m. 120-21° (HOAc and EtOH); 2-hydroxy-4-p-nitrobenzoyloxyphenyl 4-methoxybenzyl, m. 166-7° (EtOH); 2-hydroxy-4-p-toluenesulfonyloxyphenyl 4-methoxybenzyl, m. 91° (EtOH); 2,4-diacetoxyphenyl-4-nitrobenzyl, m. 157-8° (HOAc); 2,4-dibenzoyloxyphenyl 4-nitrobenzyl, m. 159-185° (HOAc); benzyl 2-hydroxy-6-methoxyphenyl, m. 66° (aqueous HOAc); benzyl 2,4,6-triacetoxyphenyl, m. 125-6° (aqueous HOAc); benzyl 2,4,6-tribenzoyloxyphenyl, m. 175° (aqueous HOAc); 4-nitrobenzyl 2,4,6-triacetoxyphenyl, m. 133-4° (aqueous HOAc); 4-nitrobenzyl 2,4,6-tribenzoyloxyphenyl, m. 126-8° (HOAc). The isoflavones were synthesized by refluxing the deoxybenzoin (1 g.) 30-60 min. with 2-3 ml. HCONH2 (A) in N or with 1.5 g. formanilide (B) at 250° and purifying by crystallization. The isoflavones prepared this way were: 5,7-dimethoxy-4-nitro-, 15% (A), 25% (B), m. 220° (C6H6); 7-methoxy-4-nitro-, 25% (A), 35% (B), m. 245° (Me2CO); 7-benzyloxy-3,4-methylenedioxy-, 25% (A), m. 168° (EtOH-HOAc); 7-methoxy-, 30% (A), m. 155-6° (MeOH); 7-benzyloxy-4-methoxy-, 30% (A), m. 182° (EtOH and EtOAc); 7-hydroxy-, 40% (B), m. 208-10° (aqueous HOAc); 7-benzyloxy-, 45% (A), m. 171° (EtOH); 4-methoxy-7-p-toluenesulfonyloxy-, 50% (B), m. 168° (C6H6); 6-methoxy-, 50% (B), m. 174° (COMe2 and HOAc); 7-hydroxy-4-methoxy- 60% (B), m. 253-4° (aqueous HOAc); and 7-p-toluenesulfonyloxy-, 60% (B), m. 212-13° (aqueous HOAc). A list of deoxybenzoins which did not yield isoflavones with (A) or (B) is given. When 2-acyloxydeoxybenzoins were heated at 250° there resulted the corresponding 2-substituted isoflavones. In this manner was prepared: 8% 7-benzyloxy-2-phenylisoflavone, m. 185-6° (EtOH); 40% 7-acetoxy-2-methylisoflavone, m. 162° (C6H6); 50% 5,7-diacetoxy-2-methyl-4-nitroisoflavone, m. 190° (EtOH-Me2CO); and 60% 7-acetoxy-2-methyl-4-nitroisoflavone, m. 245° (Me2CO).

L4 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1958:50581 HCAPLUS
DOCUMENT NUMBER: 52:50581
ORIGINAL REFERENCE NO.: 52:9097g-i,9098a-d
TITLE: Examples of very facile Baker-Venkataraman transformations
AUTHOR(S): Gupta, V. N.; Seshadri, T. R.
CORPORATE SOURCE: Delhi Univ.
SOURCE: Journal of Scientific & Industrial Research (1957), 16B, 116-19

CODEN: JSIRAC; ISSN: 0022-4456
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:50581

AB Acyl esters of 2-hydroxydeoxybenzoins undergo the Baker-Venkataraman transformation with great facility in boiling aqueous Na2CO3 or boiling acetone and anhydrous K2CO3. The increased rate of reaction is attributed to the enhanced reactivity of the methylene group. To 5 g. 2,4-dihydroxy-4'-methoxydeoxybenzoin in 20 ml. Ac2O a drop of HClO4 was added and the mixture left at room temperature 0.5 hr. H2O was added and the solid filtered off and crystallized from MeOH yielding 5 g. 2,4-diacetoxy-4'-methoxydeoxybenzoin (I), m. 109-10° (colorless rhombahedral prisms). A similar result was obtained using the method of Mehta and Seshadri (C.A. 49, 14753f) involving AcCl and pyridine. 2-Hydroxy-4,4'-dimethoxydeoxybenzoin (10 g.) (C.A. 17, 1636) in 200 ml. anhydrous benzene was refluxed with 20 g. anhydrous AlCl3 2 hrs., the solvent distilled, and the residual complex decomposed with ice and HCl. The mixture was heated on a boiling H2O bath 0.5 hr. and then cooled in ice. The solid was directly acetylated by the Ac2O-HClO4 method. The acetate formed was crystallized from MeOH giving 3 g. 2,4,4-triacetoxydeoxybenzoin (II), flat needles, m. 135-6°. Acetylation of 2,4,6-trihydroxydeoxybenzoin (C.A. 17, 1636) and crystallization from alc. gave 2,4,6-triacetoxydeoxybenzoin (III), colorless plates, m. 118-20°. I (3 g.) in 100 ml. dry acetone was refluxed in the presence of 15 g. anhydrous K2CO3 8 hrs., the inorg. salts filtered off and washed with warm acetone, the solvent distilled from the filtrate, and the residue treated with H2O and recrystd. from EtOAc yielding 2.2 g. 7-acetoxy-4'-methoxy-2-methylisoflavone (IV), rhombohedral plates, m. 194-6°. Deacetylation of IV with alc. HCl gave 7-hydroxy-4'-methoxy-2-methylisoflavone, prisms, m. 280-2° (alc.). II (3 g.) in dry acetone was refluxed in the presence of anhydrous K2CO3 8 hrs. and the product worked up as above. Crystallization from alc. gave 2 g. 7,4'-diacetoxy-2-methylisoflavone (V), thick rectangular plates, m. 194-5°. Deacetylation of V gave 7,4'-dihydroxy-2-methylisoflavone, thin rectangular plates, m. 314-15°. 2,4-Dihydroxydeoxybenzoin (5 g.) (C.A. 17, 1636) in 100 ml. dry acetone was refluxed with 7 ml. BzCl in the presence of 20 g. anhydrous K2CO3 8 hrs. and crystallized from alc. yielding 3.6 g. 7-benzoyloxy-2,3-diphenylchromone (VI), elongated rectangular prisms, m. 185-6°. VI in 8% alc. KOH was refluxed 0.5 hr., the solvent distilled in vacuo, the residue diluted with H2O, acidified, filtered, the residue repeatedly washed with boiling H2O to remove BzOH, and the water-insol. portion crystallized from alc. gave a product presumed to be 7-hydroxy-2,3-diphenylchromone, thin rectangular plates, m. 269-71°, acetylated by Ac2O-HClO4 to 7-acetoxy-2,3-diphenylchromone, prisms, m. 208-9° (alc.). III (2 g.) in 80 ml. 10% aqueous Na2CO3 was refluxed 2 hrs., cooled, acidified, and the precipitated isoflavone crystallized from alc. yielding 1.2 g. product believed to be 5,7-dihydroxy-2-methylisoflavone, pale yellowish brown prisms, m. 228°.

L4 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1957:43325 HCAPLUS
DOCUMENT NUMBER: 51:43325
ORIGINAL REFERENCE NO.: 51:8082h-i,8083a-g
TITLE: 3-Aroylbenzofurans
AUTHOR(S): Whalley, W. B.; Lloyd, G.
CORPORATE SOURCE: Univ. Liverpool, UK
SOURCE: Sci. Proc. Roy. Dublin Soc. (1956), 27, 105-10

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB 3-Aroylbenzofurans were synthesized and investigated and 2'-hydroxydeoxybenzoins prepared from isoflavones underwent spontaneous cyclization to the corresponding 2-arylbenzofurans. Demethylation of 2',7-dimethoxyisoflavone with AlCl3 gave 2'-hydroxy-7-methoxyisoflavone (I), the orientation established by ethylation to the 2'-ethoxy-I, which was also synthesized by the Na-HCO2Et cyclization of 2'-ethoxy-2-hydroxy-4-methoxydeoxybenzoin. Benzylation of I gave the 2'-benzyloxy derivative of I which gave 2'-benzyloxy-2-hydroxy-4-methoxydeoxybenzoin, which was methylated to the 2,4-di-Me derivative and converted catalytically to 2-(2',4'-dimethoxyphenyl)benzofuran. Attempts to synthesize 2,4-dimethoxybenzyl alc. or bromide gave polymeric materials only and the claims of Jacobs and Heidelberger (C.A. 9, 1610) were not substantiated. 2',5,7-Trimethoxyisoflavone was partially demethylated to 2',5-dihydroxy-7-methoxyisoflavone (II) and benzoylated to the 2-benzoyloxy derivative of II, which was methylated to 2'-benzoyloxy-5,7-dimethoxyisoflavone (III) and debenzoylated to 2'-hydroxy-5,7-dimethoxyisoflavone (IV). Orientation was established by ethylation to the 2'-ethoxy derivative of IV. Alkaline degradation of III gave 2'-benzoyloxy-2-hydroxy-4,6-dimethoxybenzoin which was methylated to the 2,4,6-tri-MeO derivative, debenzoylation of which gave 2-(2',4',6'-trimethoxyphenyl)benzofuran. Only 2-hydroxy-2',3',4,6-tetramethoxy- (V) and 2-hydroxy-2',4,4',6'-tetramethoxydeoxybenzoins of several tried furnished the expected phenoxyacetates, i.e., Et 2-(2',3',4,6-tetramethoxybenzoin)phenoxyacetate (VI), the corresponding acid, and 3-benzyl-4,6-dimethoxybenzofurans (VII). The CH2 group uniting the two ring systems in VI was not oxidized to carbonyl with SeO2 or Cr2O3, neither was V cyclized with retention of CO2H or CO2R. The formation of small quantities of VII in the condensation of BrCH2CO2Et (VIII) and V was attributed to the hydrolysis of a portion of VI and cyclization accompanied by decarboxylation. In like manner, the only product isolated from the reaction of VIII and 2-hydroxy-3',4,4',6-tetramethoxydeoxybenzoin was a small quantity of what was considered to be, by analogy, 3-(3'-4'-dimethoxybenzyl)-4,6-dimethoxybenzofuran, while 4,4',6,-trimethoxydeoxybenzoin gave a low yield of a lactone. Condensation of ethoxalyl chloride with 2-hydroxy-2',4-dimethoxybenzoin gave a low yield of 2-ethoxycarbonyl-2-hydroxy-2',7-dimethoxyisoflavonone which was simultaneously dehydrated and partially demethylated to 7'-methoxychromono(2',3',3,4)coumarin, the latter with dilute alkali gave 3-(2'-hydroxy-4'-methoxybenzoyl)benzofuran-2-carboxylic acid (IX) which was converted to the Me ester which gave 2-(2',4'-dimethoxyphenyl)benzofuran with alkali. 5',7'-Dihydroxychromono(2',3',3,4)coumarin was converted to 5',7'-dimethoxychromono(2',3',3,4)coumarin which was converted successively to 3-(2',4',6'-trimethoxybenzoyl)benzofuran-2-carboxylic acid (X) and the Me ester, followed by decarboxylation to 3-(2',4',6'-trimethoxybenzoyl)benzofuran (XI). In a similar manner, 7-methoxy-3-(2',4',6'-trimethoxybenzoyl)benzofuran was prepared from 5',7',8-trimethoxychromono(2',3',3,4)coumarin. XI, the 7-MeO analog, and 2-phenylbenzofurans were very sensitive to acids and yielded HCO2H and the appropriate 2'-hydroxy-2-methoxydeoxybenzoin with alkali and upon neutralization were spontaneously dehydrated to the corresponding 2-phenylbenzoin. XI with very mild treatment with HI gave II, while AlCl3 in PhNO2 gave a small yield of 3-(2'-hydroxy-4'-6'-dimethoxybenzoyl)benzofuran (XII) which was converted to XI together with much IV. Decarboxylation of 3-(2'-hydroxy-4',6'-dimethoxybenzoyl)benzofuran-2-carboxylic acid (XIII) in boiling quinoline gave a low yield of XII and much IV, since the conversion of such benzofurans to isoflavones was acid-base catalyzed. IX, X, and

XIII underwent almost quantitative conversion to the corresponding chromono(2',3',3,4)coumarins (XIV). A consideration of the general properties of XIV substantiated the formulation of these rotenononic acid analogs, and rotenononic acid itself, as derivs. of 3-aroylbenzofuran.

L4 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1956:69288 HCAPLUS
DOCUMENT NUMBER: 50:69288
ORIGINAL REFERENCE NO.: 50:12928d-i,12929a
TITLE: Deoxybenzoins. II. γ-Deoxybenzoins
AUTHOR(S): Libermann, David; Moyeux, Maurice
CORPORATE SOURCE: Theraplix, Montrouge, Seine
SOURCE: Bulletin de la Societe Chimique de France (1956) 166-73
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 47, 2152f. Treating 3.5 g. PhCH2CN, 6.35 g. 4-cyclohexylresorcinol, and 3.5 g. anhydrous ZnCl2 in 60 cc. anhydrous Et2O cooled in ice, with HCl 5 h. gave a solid and a liquid ketimine, which are boiled sep. 1 h. with 100 cc. H2O and 10 cc. NH4OH to yield, resp., 2,4-dihydroxy-(I) (β-isomer), m. 133° (from C6H6-ligroine) and 2,6-dihydroxy-5-cyclohexyldeoxybenzoin (II) (γ-isomer), green, m. 221° (from alc.). Heated 8 h. at 170-80° with 10 cc. Ac2O and 2 g. anhydrous NaOAc, 1 g. I gives 2-methyl-7-acetoxy-6-cyclohexylisoflavone, m. 131-2° (from alc.). Treated similarly, II gives the triacetate (monohydrate from alc., m. 165°), which, heated 3 h. with 10% NaOH and acidified, gives α-acetyl-2,6-dihydroxy-5-cyclohexyldeoxybenzoin, m. 142°. The "2,4-dihydroxydeoxybenzoin," m. 115° (III) of Badcock, et al. (C.A. 45, 6177a), is shown to be a mixture of 85% 2,4-(IV), m. 118°, and 15% 2,6-dihydroxydeoxybenzoin (V), m. 177°. Distillation of III yields IV, b0.2 192-4°; di-Me ether, m. 53°; oxime, m. 240°. V is obtained from the mother liquor in crystallizing III. Et2NCH2CH2Cl (VI) (89 g.) is added to 74.8 g. III and 15.1 g. Na cooled in 200 cc. absolute EtOH, the mixture refluxed 4 h., filtered, evaporated, the residue treated with 300 cc. H2O and HCl to pH 2-3, extracted with Et2O, and the extract on evaporation gives 5 g. 2-vinyloxy-6-hydroxydeoxybenzoin (VII), m. 85° (alc.); phenylurethane, m. 130°; oxime, m. 173°. The aqueous solution is made alkaline and extracted 3 times with Et2O. The extract contains an emulsion of 10 g. [2,3-PhCH2CO(HO)C6H3OCH2CH2NEt2CH2CH2NEt2]OH which is separated The extract is then evaporated and the residue extracted with boiling H2O to remove 3 g. (Et2NCH2)2, b. 173-7°, leaving 81 g. 2,4-(Et2NCH2CH2O)2C6H3COCH2Ph (VIII), b0.2 192-3°; dioxalate, m. 151°. 4-RC6H4CH2COC6H3(OCH:CH2)OH-2,6 (IX) are isolated from similar reactions of VI with the 4-RC6H4CH2COC6H3(OH)2-2,4 (X) made by condensing p-RC6H4CH2COCl with m-C6H4(OH)2(R and m.p. of IX and X given): Cl, -, 156°; Br, 103°, 176°; I, 131°, 186°. With Me2SO4, VII gives the Me ether, m. 73°; oxime, m. 143°. Hydrogenation of VII gives 2-ethoxy-6-hydroxydeoxybenzoin (XI), m. 82°; oxime, m. 178°. Heated with Ac2O and NaOAc, XI, VII, and 4-ethoxy-2-hydroxydeoxybenzoin, m. 86°, give 5-ethoxy-2-methyl-, m. 179-80°, 5-vinyloxy-2-methyl-, m. 173°, and 7-ethoxy-2-methylisoflavone, m. 136°, resp. Treated similarly, III gives 2-methyl-7-acetoxyisoflavone, m. 165°, and 2,6-dihydroxybenzoin triacetate, m. 210°. With Br in HOAc, VII

gives the dibromide, m. 147°; heated with AlCl3, VII yields V, and with iodine in pyridine (King and McWirther, C.A. 40, 3417.5), VII gives 40% 2,6-EtO(MeO)C6H3CO2H, m. 128°. Similarly, 2,4-dimethoxydeoxybenzoin gives dimethyl-β-resorcylic acid, m. 107°. With KMnO4 in aqueous pyridine, VII gives 2,5-dihydroxy-2-hydroxymethylisoflavanone, m. 111°, and 2,5-dihydroxyisoflavanone-2-carboxylic acid, m. 205° (decomposition).

L4 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1956:1504 HCAPLUS
DOCUMENT NUMBER: 50:1504
ORIGINAL REFERENCE NO.: 50:323i,324a
TITLE: A new synthesis of isoflavones and of other chromones
AUTHOR(S): Gowan, J. E.; O'Connor, N. S.; Wheeler, T. S.
CORPORATE SOURCE: .Univ. Coll., Dublin, Ire.
SOURCE: Chemistry & Industry (London, United Kingdom) (1954) 1201
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Isoflavones were synthesized from HCONH2 (I) and 2-hydroxydeoxybenzoins. 2-Hydroxydeoxybenzoin and I refluxed 1 hr., and the mixture poured into H2O yielded isoflavone (II), which recrystd. from EtOH gave a material which did not depress the m.p. of an authentic sample of II. 7-Methoxyisoflavone and 7-benzyloxy-4'-methoxyisoflavone were similarly obtained in 30% yield from 4,2-MeO(HO)C6H3COCH2Ph and 4,2-PhCH2O(HO)C6H3COCH2C6H4OMe-4, resp. The yield was not improved by the addition of either H2SO4 or HCO2H. Flavone was prepared similarly from BzNH2 and 2-HOC6H4Ac.

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L6 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:80674 HCAPLUS
DOCUMENT NUMBER: 140:128190
TITLE: Process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivatives
INVENTOR(S): Burdet, Bruno; Ruettimann, August
PATENT ASSIGNEE(S): Roche Vitamins Ag, Switz.; DSM IP Assets B.V.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009576	A2	20040129	WO 2003-EP7575	20030714
WO 2004009576	A3	20040513		

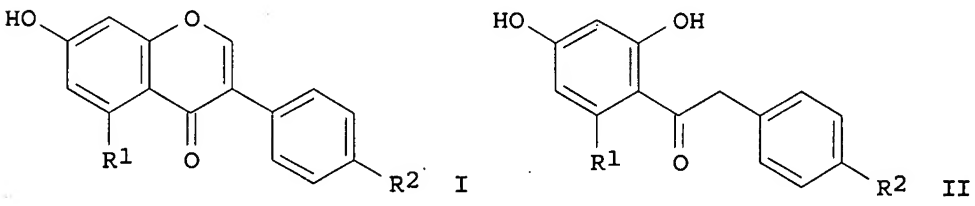
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ,

UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2492201	A1	20040129	CA 2003-2492201	20030714
AU 2003254341	A1	20040209	AU 2003-254341	20030714
EP 1523478	A2	20050420	EP 2003-764976	20030714
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003012840	A	20050426	BR 2003-12840	20030714
CN 1684950	A	20051019	CN 2003-817676	20030714
JP 2005534682	T	20051117	JP 2004-522445	20030714
MX 2005PA00795	A	20050419	MX 2005-PA795	20050119
US 2005256321	A1	20051117	US 2005-521972	20050121
PRIORITY APPLN. INFO.:			EP 2002-16494 A	20020723
			WO 2003-EP7575 W	20030714

OTHER SOURCE(S): CASREACT 140:128190; MARPAT 140:128190

GI



AB The present invention discloses a process for manufacturing hydroxylated isoflavone derivs., such as I [R1 = H, OH; R2 = OH, alkoxy] by reacting an appropriately substituted 2-hydroxydeoxybenzoin derivs. II with formic acid anhydride, HCOOCOR3 [R3 = alkyl, haloalkyl, alkoxymethyl, carboxyalkyl, arylalkyl, cycloalkyl, aryl, heteroaryl, aminoalkyl, alkoxy, aryloxy], in the presence of a base or in a solvent which acts as a base, and if necessary promoting the ensuing hydrolysis of the so-produced acylated form of I by acidification. Of particular interest as products of this process are the 5,7-dihydroxyisoflavones, e.g. genistein I [R1, R2 = OH (III)]. Thus, propionyl formic anhydride, formed by the reaction of sodium formate and propionyl chloride, was reacted with II [R1, R2 = OH], and the product was hydrolyzed to afford III of 98.9% purity. Isoflavones display many useful biochem. effects.

=> d l7 ibib abs hitstr tot

L7 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:80674 HCAPLUS
DOCUMENT NUMBER: 140:128190
TITLE: Process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivatives
INVENTOR(S): Burdet, Bruno; Ruettimann, August
PATENT ASSIGNEE(S): Roche Vitamins Ag, Switz.; DSM IP Assets B.V.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009576	A2	20040129	WO 2003-EP7575	20030714
WO 2004009576	A3	20040513		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2492201	A1	20040129	CA 2003-2492201	20030714
AU 2003254341	A1	20040209	AU 2003-254341	20030714
EP 1523478	A2	20050420	EP 2003-764976	20030714
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003012840	A	20050426	BR 2003-12840	20030714
CN 1684950	A	20051019	CN 2003-817676	20030714
JP 2005534682	T	20051117	JP 2004-522445	20030714
MX 2005PA00795	A	20050419	MX 2005-PA795	20050119
US 2005256321	A1	20051117	US 2005-521972	20050121
PRIORITY APPLN. INFO.:			EP 2002-16494 A	20020723
			WO 2003-EP7575 W	20030714

OTHER SOURCE(S): CASREACT 140:128190; MARPAT 140:128190
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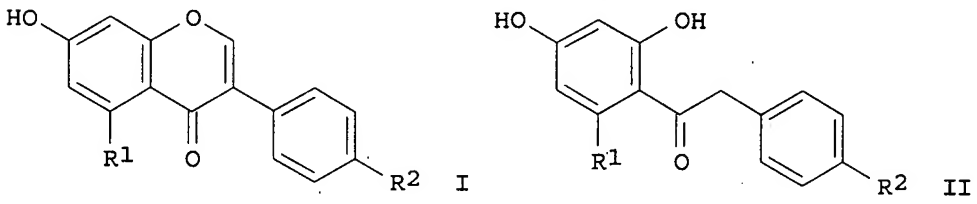
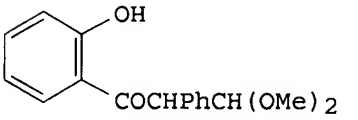
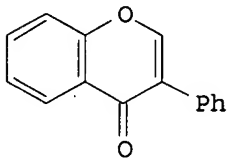


AB The present invention discloses a process for manufacturing hydroxylated isoflavone derivs., such as I [R1 = H, OH; R2 = OH, alkoxy] by reacting an appropriately substituted 2-hydroxydeoxybenzoin derivs. II with formic acid anhydride, HCOOCOR3 [R3 = alkyl, haloalkyl, alkoxymethyl, carboxyalkyl, arylalkyl, cycloalkyl, aryl, heteroaryl, aminoalkyl, alkoxy, aryloxy], in the presence of a base or in a solvent which acts as a base , and if necessary promoting the ensuing hydrolysis of the so-produced acylated form of I by acidification. Of particular interest as products of this process are the 5,7-dihydroxyisoflavones, e.g. genistein I [R1, R2 = OH (III)]. Thus, propionyl formic anhydride, formed by the reaction of sodium formate and propionyl chloride, was reacted with II [R1, R2 = OH], and the product was hydrolyzed to afford III of 98.9% purity. Isoflavones display many useful biochem. effects.

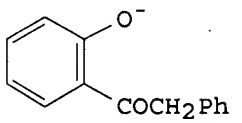
L7 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:441861 HCAPLUS
DOCUMENT NUMBER: 89:41861
TITLE: Base-catalyzed transformation of a β-dicarbonyl acetal, 1-(2-hydroxyphenyl)-2-phenyl-3,3-dimethoxypropan-1-one into isoflavone and 2-hydroxydeoxybenzoin
AUTHOR(S): Zsuga, M.; Szabo, V.; Balogh, L.
CORPORATE SOURCE: Inst. Appl. Chem., Lajos Kossuth Univ., Debrecen, Hung.
SOURCE: Reaction Kinetics and Catalysis Letters (1978), 8(1), 1-6
CODEN: RKCLAU; ISSN: 0133-1736
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II



III

AB The decomposition of I depends on the OH- concentration At [OH-] ≤10-3M. I transforms into II, while at [OH-] = 10-2M, it decomps. to III via an enol-enolate equilibrium These unusual base-catalyzed transformations are explained by the high mobility of the α-proton of I, and by the stability of II towards nucleophilic reagents.

L7 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1957:43325 HCAPLUS
DOCUMENT NUMBER: 51:43325
ORIGINAL REFERENCE NO.: 51:8082h-i,8083a-g
TITLE: 3-Aroylbenzofurans
AUTHOR(S): Whalley, W. B.; Lloyd, G.
CORPORATE SOURCE: Univ. Liverpool, UK
SOURCE: Sci. Proc. Roy. Dublin Soc. (1956), 27, 105-10
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB 3-Aroylbenzofurans were synthesized and investigated and 2'-hydroxydeoxybenzoins prepared from isoflavones underwent spontaneous cyclization to the corresponding 2-arylbenzofurans. Demethylation of 2',7-dimethoxyisoflavone with AlCl3 gave 2'-hydroxy-7-methoxyisoflavone (I), the orientation established by ethylation to the 2'-ethoxy-I, which was also synthesized by the Na-HCO2Et cyclization of 2'-ethoxy-2-hydroxy-4-methoxydeoxybenzoin. Benzylation of I gave the 2'-benzyloxy derivative of I which gave 2'-benzyloxy-2-hydroxy-4-methoxydeoxybenzoin, which was methylated to the 2,4-di-Me derivative and converted catalytically to 2-(2',4'-dimethoxyphenyl)benzofuran. Attempts to synthesize 2,4-dimethoxybenzyl alc. or bromide gave polymeric materials

only and the claims of Jacobs and Heidelberger (C.A. 9, 1610) were not substantiated. 2',5,7-Trimethoxyisoflavone was partially demethylated to 2',5-dihydroxy-7-methoxyisoflavone (II) and benzoylated to the 2-benzoyloxy derivative of II, which was methylated to 2'-benzoyloxy-5,7-dimethoxyisoflavone (III) and debenzoylated to 2'-hydroxy-5,7-dimethoxyisoflavone (IV). Orientation was established by ethylation to the 2'-ethoxy derivative of IV. Alkaline degradation of III gave 2'-benzoyloxy-2-hydroxy-4,6-dimethoxybenzoin which was methylated to the 2,4,6-tri-MeO derivative, debenzoylation of which gave 2-(2',4',6'-trimethoxyphenyl)benzofuran. Only 2-hydroxy-2',3',4,6-tetramethoxy- (V) and 2-hydroxy-2',4,4',6'-tetramethoxydeoxybenzoins of several tried furnished the expected phenoxyacetates, i.e., Et 2-(2',3',4,6-tetramethoxybenzoin)phenoxyacetate (VI), the corresponding acid, and 3-benzyl-4,6-dimethoxybenzofurans (VII). The CH2 group uniting the two ring systems in VI was not oxidized to carbonyl with SeO2 or Cr2O3, neither was V cyclized with retention of CO2H or CO2R. The formation of small quantities of VII in the condensation of BrCH2CO2Et (VIII) and V was attributed to the hydrolysis of a portion of VI and cyclization accompanied by decarboxylation. In like manner, the only product isolated from the reaction of VIII and 2-hydroxy-3',4,4',6-tetramethoxydeoxybenzoin was a small quantity of what was considered to be, by analogy, 3-(3'-4'-dimethoxybenzyl)-4,6-dimethoxybenzofuran, while 4,4',6,-trimethoxydeoxybenzoin gave a low yield of a lactone. Condensation of ethoxalyl chloride with 2-hydroxy-2',4-dimethoxybenzoin gave a low yield of 2-ethoxycarbonyl-2-hydroxy-2',7-dimethoxyisoflavonone which was simultaneously dehydrated and partially demethylated to 7'-methoxychromono(2',3',3,4)coumarin, the latter with dilute alkali gave 3-(2'-hydroxy-4'-methoxybenzoyl)benzofuran-2-carboxylic acid (IX) which was converted to the Me ester which gave 2-(2',4'-dimethoxyphenyl)benzofuran with alkali. 5',7'-Dihydroxychromono(2',3',3,4)coumarin was converted to 5',7'-dimethoxychromono(2',3',3,4)coumarin which was converted successively to 3-(2',4',6'-trimethoxybenzoyl)benzofuran-2-carboxylic acid (X) and the Me ester, followed by decarboxylation to 3-(2',4',6'-trimethoxybenzoyl)benzofuran (XI). In a similar manner, 7-methoxy-3-(2',4',6'-trimethoxybenzoyl)benzofuran was prepared from 5',7',8-trimethoxychromono(2',3',3,4)coumarin. XI, the 7-MeO analog, and 2-phenylbenzofurans were very sensitive to acids and yielded HCO2H and the appropriate 2'-hydroxy-2-methoxydeoxybenzoin with alkali and upon neutralization were spontaneously dehydrated to the corresponding 2-phenylbenzoin. XI with very mild treatment with HI gave II, while AlCl3 in PhNO2 gave a small yield of 3-(2'-hydroxy-4'-6'-dimethoxybenzoyl)benzofuran (XII) which was converted to XI together with much IV. Decarboxylation of 3-(2'-hydroxy-4',6'-dimethoxybenzoyl)benzofuran-2-carboxylic acid (XIII) in boiling quinoline gave a low yield of XII and much IV, since the conversion of such benzofurans to isoflavones was acid-base catalyzed.
IX, X, and XIII underwent almost quantitative conversion to the corresponding chromono(2',3',3,4)coumarins (XIV). A consideration of the general properties of XIV substantiated the formulation of these rotenononic acid analogs, and rotenononic acid itself, as derivs. of 3-aroylbenzofuran.

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=> s hydroxylated isoflavone
        17955 HYDROXYLATED
         6562 ISOFLAVONE
         5686 ISOFLAVONES
         8261 ISOFLAVONE
                (ISOFLAVONE OR ISOFLAVONES)
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L8            5 HYDROXYLATED ISOFLAVONE
                (HYDROXYLATED(W)ISOFLAVONE)

=> s l8 and 2-hydroxydeoxybenzoin
        9272756 2
             57 HYDROXYDEOXYBENZOIN
             26 HYDROXYDEOXYBENZOINS
             67 HYDROXYDEOXYBENZOIN
                  (HYDROXYDEOXYBENZOIN OR HYDROXYDEOXYBENZOINS)
             21 2-HYDROXYDEOXYBENZOIN
                  (2(W)HYDROXYDEOXYBENZOIN)
L9            1 L8 AND 2-HYDROXYDEOXYBENZOIN

=> d l8 ibib abs hitstr tot

L8   ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2006:1123428  HCAPLUS
DOCUMENT NUMBER:          145:438449
TITLE:                    Process for the manufacture of hydroxylated
                          isoflavones
INVENTOR(S):              Ruettimann, August; Stangl, Jochen
PATENT ASSIGNEE(S):       DSM IP Assets B.V., Neth.
SOURCE:                   PCT Int. Appl., 16pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
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     WO 2006111289         A1    20061026    WO 2006-EP3252           20060410
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:                          EP 2005-8389        A  20050418
OTHER SOURCE(S):          CASREACT 145:438449; MARPAT 145:438449
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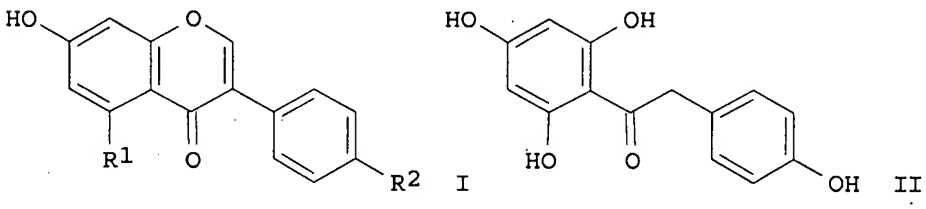


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AB   A process was disclosed for the preparation of hydroxylated
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isoflavones, such as I [R1 = H, OH; R2 = OH, C1-6-alkoxy], by reacting in a Hoesch reaction using an alkanoic acid alkyl ester as solvent a phenol with a phenylacetonitrile to yield a 1,2-diphenylethanone and transforming the ethanone into an isoflavone by well-known methods. Thus, α-(p-hydroxyphenyl)phloroacetophenone (II) was prepared with 64% yield by reacting phloroglucinol with HO-4-C6H4CH2CN using gaseous HCl in MeCO2Et for 60 min, adjusting the pH of the reaction mixture to 4.0 using aqueous NaOH, heating the solution to 75° and adding MeCO2Et and refluxing the mixture for 5 h. Genistein I (R1 = R2 = OH) was then prepared by a cyclization reaction with 91.7% yield of II with sodium formate and MeCOCl in Me2CO at 12-15° under Ar, stirring at 23-25° for 2 h, treatment with Et3N at 18-20° and adding 38% H2SO4.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:80674 HCAPLUS
DOCUMENT NUMBER: 140:128190
TITLE: Process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivatives
INVENTOR(S): Burdet, Bruno; Ruettimann, August
PATENT ASSIGNEE(S): Roche Vitamins Ag, Switz.; DSM IP Assets B.V.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009576	A2	20040129	WO 2003-EP7575	20030714
WO 2004009576	A3	20040513		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2492201	A1	20040129	CA 2003-2492201	20030714
AU 2003254341	A1	20040209	AU 2003-254341	20030714
EP 1523478	A2	20050420	EP 2003-764976	20030714
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003012840	A	20050426	BR 2003-12840	20030714
CN 1684950	A	20051019	CN 2003-817676	20030714
JP 2005534682	T	20051117	JP 2004-522445	20030714
MX 2005PA00795	A	20050419	MX 2005-PA795	20050119
US 2005256321	A1	20051117	US 2005-521972	20050121

PRIORITY APPLN. INFO.: EP 2002-16494 A 20020723
WO 2003-EP7575 W 20030714

OTHER SOURCE(S): CASREACT 140:128190; MARPAT 140:128190
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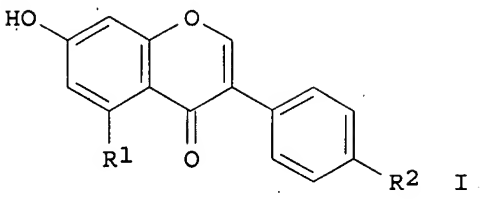

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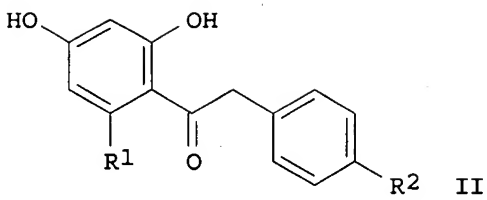


II

AB The present invention discloses a process for manufacturing hydroxylated isoflavone derivs., such as I [R1 = H, OH; R2 = OH, alkoxy] by reacting an appropriately substituted 2-hydroxydeoxybenzoin derivs. II with formic acid anhydride, HCOOCOR3 [R3 = alkyl, haloalkyl, alkoxymethyl, carboxyalkyl, arylalkyl, cycloalkyl, aryl, heteroaryl, aminoalkyl, alkoxy, aryloxy], in the presence of a base or in a solvent which acts as a base, and if necessary promoting the ensuing hydrolysis of the so-produced acylated form of I by acidification. Of particular interest as products of this process are the 5,7-dihydroxyisoflavones, e.g. genistein I [R1, R2 = OH (III)]. Thus, propionyl formic anhydride, formed by the reaction of sodium formate and propionyl chloride, was reacted with II [R1, R2 = OH], and the product was hydrolyzed to afford III of 98.9% purity. Isoflavones display many useful biochem. effects.

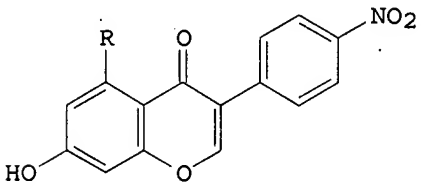
L8 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:592788 HCAPLUS
DOCUMENT NUMBER: 129:289296
TITLE: A potent antioxidative and anti-UV-B isoflavonoids transformed microbiologically from soybean components
AUTHOR(S): Mimura, Akio; Yazaki, Shin-Ichi; Tanimura, Hiroshi
CORPORATE SOURCE: Department of Biotechnology, Yamanashi University, Kofu, 400, Japan
SOURCE: ACS Symposium Series (1998), 701(Functional Foods for Disease Prevention I: Fruits, Vegetables, and Teas), 127-137
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB Japanese traditional fermented soybean foods (miso(soybean paste), soy sauce, natto and so on) were hypothesized to contribute to the lower incidence of human cancers and cardiac diseases. Soybeans were rich in isoflavonoid glucosides such as daidzin and genistin. During the fermentation with microorganisms, these glucosides could be hydrolyzed to aglycon isoflavones (daidzein and genistein), and further transformed to biol. active compds. such as more hydroxylated isoflavones.
Several kinds of fungi relating to the fermented foods and bacteria isolated from soil were screened for the production of potent activity of antioxidn. (anti-UV-B) from soybean components. Aspergillus niger IFO 4414 was selected as the most potent producer of antioxidative isoflavones. The fungus was cultivated in the medium composed of soybean flour, and it was observed that anti-UV-B activity of the culture exts. was increased remarkably during the fermentation From the fermented soybeans, a isoflavone with potent anti-UV-B activity was isolated and identified as 4',7,8-trihydroxyisoflavone (8-hydroxydaidzein), which was demonstrated as the hydroxylated product of daidzein at the 8-position of A-ring. The maximum conversion rate to 4',7,8-trihydroxyisoflavone from daidzein was 67.8%(weight/weight). 4',7,8-Trihydroxyisoflavone was observed to have almost same

anti-UV-B activity (antioxidative activity) as BHA, 60 to 100 times stronger activity than alpha-tocopherol, and about 15 times stronger activity than daidzein and genistein, using the measurement method with rabbit erythrocyte membrane ghosts irradiating UV-B light. All this and more was reviewed with 17 refs.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:6375 HCAPLUS
DOCUMENT NUMBER: 116:6375
TITLE: A facile and practical preparation of 5,7-dihydroxy-3-(4-nitrophenyl)-4H-1-benzopyran-4-one
AUTHOR(S): Liu, D. F.; Cheng, C. C.
CORPORATE SOURCE: Cancer Cent., Univ. Kansas, Kansas City, KS, 66103, USA
SOURCE: Journal of Heterocyclic Chemistry (1991), 28(6), 1641-2
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:6375
GI



I

AB In spite of the fact that several preparative methods for the synthesis of hydroxylated isoflavones were reported during the past fifty years, none is suitable for the preparation of isoflavones containing 5,7-dihydroxy functions. This paper reports a simple, large scale preparation of 5,7-dihydroxy-3-(4-nitrophenyl)-4H-1-benzopyran-4-one (I, R = OH) by the condensation of the readily available 2,4,6-(HO)3C6H2COCH2C6H4NO2-4 and acetic formic anhydride in high yields. Similar isoflavones, such as I (R = H), can also be obtained in good yields in an analogous manner.

L8 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:76357 HCAPLUS
DOCUMENT NUMBER: 74:76357
TITLE: Noel bismethylene transfer to 2'-hydroxylated isoflavones by dimethylsulfoxonium methylide: the reaction and its products
AUTHOR(S): Crombie, Leslie; Davies, John Salmon; Whiting, Donald A.
CORPORATE SOURCE: Dep. Chem., Univ. Coll. New South Wales, Cardiff, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1971), (2), 304-12
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 74:76357
GI For diagram(s), see printed CA Issue.

AB Isoderritol isoflavone (I) reacted with excess ylide Me2S(O):CH2 to give a hydroxycyclopentene (II) and by-product decarboxyisoroteno-nonic acid (III). The mechanism [ring cleavage, methylene transfer, and recyclization via the vinylcoumaranone (IV)] was discussed. Acid rearrangement of II gave the stilbenoid cyclopentenone (V), and the dihydro derivative (VI) of II gave a hexacyclic compound (VII). Derritol isoflavone reacted similarly with Me2S(O):CH2. Equimolar amts. of I and Me2S(O):CH2 gave IV.

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L9 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:80674 HCAPLUS
DOCUMENT NUMBER: 140:128190
TITLE: Process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivatives
INVENTOR(S): Burdet, Bruno; Ruettimann, August
PATENT ASSIGNEE(S): Roche Vitamins Ag, Switz.; DSM IP Assets B.V.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009576	A2	20040129	WO 2003-EP7575	20030714
WO 2004009576	A3	20040513		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2492201	A1	20040129	CA 2003-2492201	20030714
AU 2003254341	A1	20040209	AU 2003-254341	20030714
EP 1523478	A2	20050420	EP 2003-764976	20030714
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US 2005256321	A1	20051117	US 2005-521972	20050121

PRIORITY APPLN. INFO.: EP 2002-16494 A 20020723
WO 2003-EP7575 W 20030714

OTHER SOURCE(S): CASREACT 140:128190; MARPAT 140:128190
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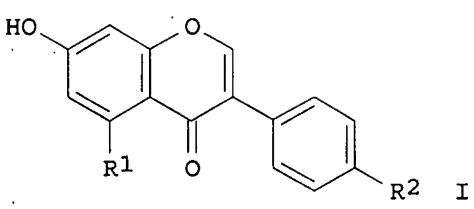

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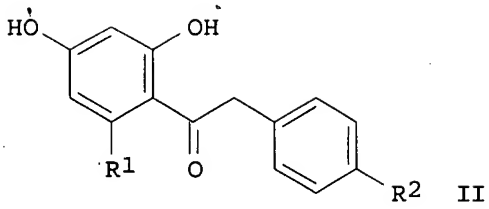

II

AB The present invention discloses a process for manufacturing hydroxylated isoflavone derivs., such as I [R1 = H, OH; R2 = OH, alkoxy] by reacting an appropriately substituted 2-hydroxydeoxybenzoin derivs. II with formic acid anhydride, HCOOCOR3 [R3 = alkyl, haloalkyl, alkoxymethyl, carboxyalkyl, arylalkyl, cycloalkyl, aryl, heteroaryl, aminoalkyl, alkoxy, aryloxy], in the presence of a base or in a solvent which acts as a base, and if necessary promoting the ensuing hydrolysis of the so-produced acylated form of I by acidification. Of particular interest as products of this process are the 5,7-dihydroxyisoflavones, e.g. genistein I [R1, R2 = OH (III)]. Thus, propionyl formic anhydride, formed by the reaction of sodium formate and propionyl chloride, was reacted with II [R1, R2 = OH], and the product was hydrolyzed to afford III of 98.9% purity. Isoflavones display many useful biochem. effects.

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	135.52	135.73

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-18.72	-18.72

STN INTERNATIONAL LOGOFF AT 12:03:13 ON 30 AUG 2007

10521972c.trn

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LOGINID:SSSPTA1626GMS

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	MAY 01	New CAS web site launched
NEWS 3	MAY 08	CA/CAplus Indian patent publication number format defined
NEWS 4	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 5	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS 6	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS 7	MAY 21	CA/CAplus enhanced with additional kind codes for German patents
NEWS 8	MAY 22	CA/CAplus enhanced with IPC reclassification in Japanese patents
NEWS 9	JUN 27	CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 10	JUN 29	STN Viewer now available
NEWS 11	JUN 29	STN Express, Version 8.2, now available
NEWS 12	JUL 02	LEMBASE coverage updated
NEWS 13	JUL 02	LMEDLINE coverage updated
NEWS 14	JUL 02	SCISEARCH enhanced with complete author names
NEWS 15	JUL 02	CHEMCATS accession numbers revised
NEWS 16	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS 17	JUL 16	CAplus enhanced with French and German abstracts
NEWS 18	JUL 18	CA/CAplus patent coverage enhanced
NEWS 19	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 20	JUL 30	USGENE now available on STN
NEWS 21	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 22	AUG 06	BEILSTEIN updated with new compounds
NEWS 23	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 24	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 25	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 26	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 27	AUG 27	USPATOLD now available on STN
NEWS 28	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that

specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:17:32 ON 30 AUG 2007

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 12:17:46 ON 30 AUG 2007
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 AUG 2007 HIGHEST RN 945828-45-5
DICTIONARY FILE UPDATES: 29 AUG 2007 HIGHEST RN 945828-45-5

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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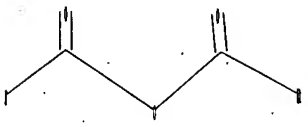
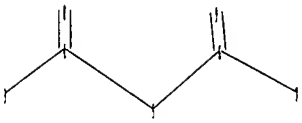
http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10521972c.str





chain nodes :
3 4 5 6 7 8 9
chain bonds :
3-4 4-5 4-8 5-6 6-7 6-9
exact/norm bonds :
4-5 4-8 5-6 6-9
exact bonds :
3-4 6-7

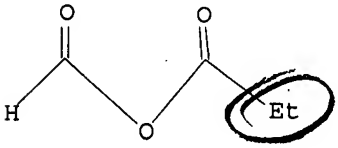
G1:H,OH

G2:OH,MeO,EtO,n-PrO,n-BuO

Match level :
3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,OH
G2 OH,MeO,EtO,n-PrO,n-BuO

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 12:18:00 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 4670 TO ITERATE

42.8% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 89302 TO 97498
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

10521972c.trn

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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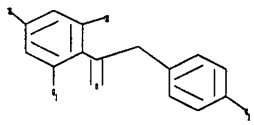
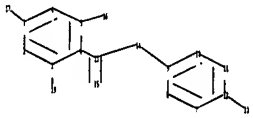
Uploading C:\Program Files\Stnexp\Queries\10521972d.str





chain nodes :
13 14 15 16 17 19 21
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
1-19 3-17 5-16 6-13 9-14 12-21 13-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-19 3-17 5-16 12-21 13-15
exact bonds :
6-13 9-14 13-14
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 : 7 :

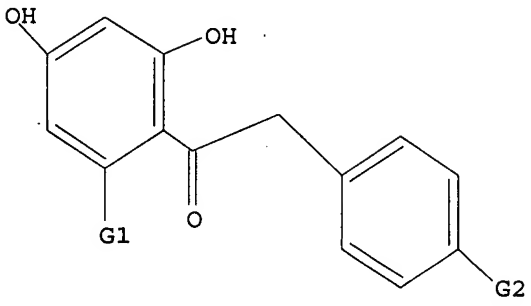
G1:H,OH

G2:OH,MeO,EtO,n-PrO,n-BuO

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:CLASS
21:CLASS

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR



G1 H,OH
G2 OH,MeO,EtO,n-PrO,n-BuO

Structure attributes must be viewed using STN Express query preparation.

=> s l5
SAMPLE SEARCH INITIATED 12:20:30 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 114 TO ITERATE

100.0% PROCESSED 114 ITERATIONS 11 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1640 TO 2920
PROJECTED ANSWERS: 22 TO 418

L6 11 SEA SSS SAM L5

=> s l5 sss full
FULL SEARCH INITIATED 12:20:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2501 TO ITERATE

100.0% PROCESSED 2501 ITERATIONS 201 ANSWERS
SEARCH TIME: 00.00.01

L7 201 SEA SSS FUL L5

=> FIL HCAPLUS
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	352.21

FILE 'HCAPLUS' ENTERED AT 12:20:43 ON 30 AUG 2007
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FILE COVERS 1907 - 30 Aug 2007 VOL 147 ISS 10
FILE LAST UPDATED: 29 Aug 2007 (20070829/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l7
L8 575 L7
=> d his

(FILE 'HOME' ENTERED AT 12:17:32 ON 30 AUG 2007)

FILE 'REGISTRY' ENTERED AT 12:17:46 ON 30 AUG 2007
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 1 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 12:18:34 ON 30 AUG 2007
L4 9 S L3

FILE 'REGISTRY' ENTERED AT 12:20:05 ON 30 AUG 2007
L5 STRUCTURE UPLOADED
L6 11 S L5
L7 201 S L5 SSS FULL

FILE 'HCAPLUS' ENTERED AT 12:20:43 ON 30 AUG 2007
L8 575 S L7

=> s l4 and l8
L9 1 L4 AND L8

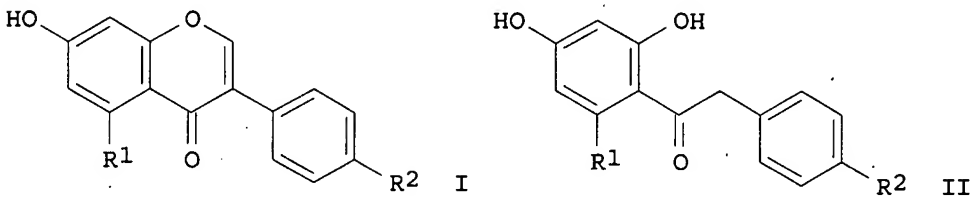
=> d l9 ibib abs hitstr tot

L9 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:80674 HCAPLUS
DOCUMENT NUMBER: 140:128190
TITLE: Process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivatives
INVENTOR(S): Burdet, Bruno; Ruettimann, August
PATENT ASSIGNEE(S): Roche Vitamins Ag, Switz.; DSM IP Assets B.V.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004009576	A2	20040129	WO 2003-EP7575		20030714
WO 2004009576	A3	20040513			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2492201	A1	20040129	CA 2003-2492201		20030714
AU 2003254341	A1	20040209	AU 2003-254341		20030714
EP 1523478	A2	20050420	EP 2003-764976		20030714
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
BR 2003012840	A	20050426	BR 2003-12840		20030714
CN 1684950	A	20051019	CN 2003-817676		20030714
JP 2005534682	T	20051117	JP 2004-522445		20030714
MX 2005PA00795	A	20050419	MX 2005-PA795		20050119
US 2005256321	A1	20051117	US 2005-521972		20050121
PRIORITY APPLN. INFO.:			EP 2002-16494	A	20020723
			WO 2003-EP7575	W	20030714

OTHER SOURCE(S): CASREACT 140:128190; MARPAT 140:128190

GI

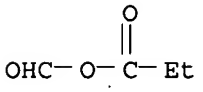


AB The present invention discloses a process for manufacturing hydroxylated isoflavone derivs., such as I [R1 = H, OH; R2 = OH, alkoxy] by reacting an appropriately substituted 2-hydroxydeoxybenzoin derivs. II with formic acid anhydride, HCOOCOR3 [R3 = alkyl, haloalkyl, alkoxymethyl, carboxyalkyl, arylalkyl, cycloalkyl, aryl, heteroaryl, aminoalkyl, alkoxy, aryloxy], in the presence of a base or in a solvent which acts as a base, and if necessary promoting the ensuing hydrolysis of the so-produced acylated form of I by acidification. Of particular interest as products of this process are the 5,7-dihydroxyisoflavones, e.g. genistein I [R1, R2 = OH (III)]. Thus, propionyl formic anhydride, formed by the reaction of sodium formate and propionyl chloride, was reacted with II [R1, R2 = OH], and the product was hydrolyzed to afford III of 98.9% purity. Isoflavones display many useful biochem. effects.

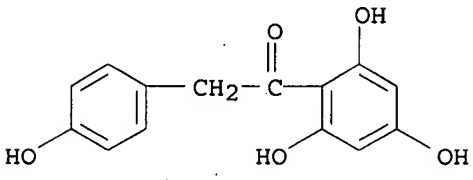
IT 10500-31-9P, Propionyl formic anhydride
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivs.)

RN 10500-31-9 HCAPLUS

CN Formic acid, anhydride with propanoic acid (CA INDEX NAME)



IT 15485-65-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivs.)
RN 15485-65-1 HCAPLUS
CN Ethanone, 2-(4-hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)- . (CA INDEX NAME)



=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	26.07	378.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.78	-0.78

STN INTERNATIONAL LOGOFF AT 12:25:45 ON 30 AUG 2007